

Mathematical Foundations of Reinforcement Learning

Markov decision processes: basics



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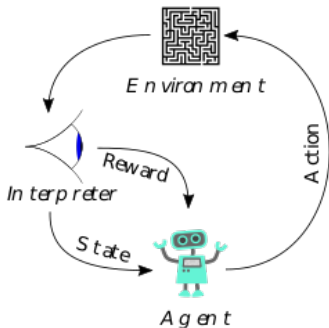
Outline

Markov decision processes

Policy evaluation

Reinforcement learning

In reinforcement learning (RL), an agent learns through interaction with the (unknown) environment.



RL has deep connection with control theory, and is also sometimes called **approximate dynamic programming**. It can be viewed as a type of **optimal control theory** with no pre-defined model of the environment.

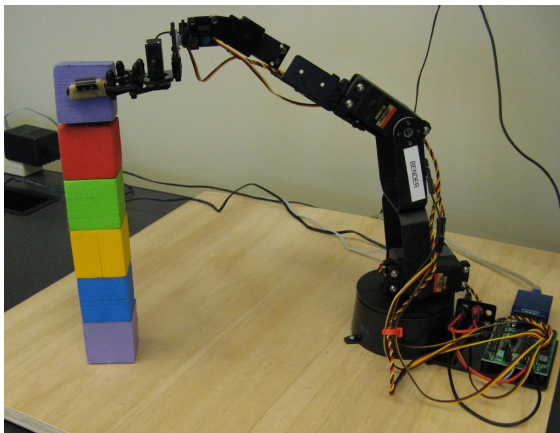
Applications of RL

RL can be applied to many different areas.

- **Robotics**: in which direction and how fast should a robot arm move?
- **Mobility**: where should taxis go to pick up passengers?
- **Transportation**: when should traffic lights turn green?
- **Recommendations**: which news stories will users click on?
- **Network configuration**: which parameter settings lead to the best allocation of resources?

Similar to multi-armed bandits, but with a notion of **state** or **context**.

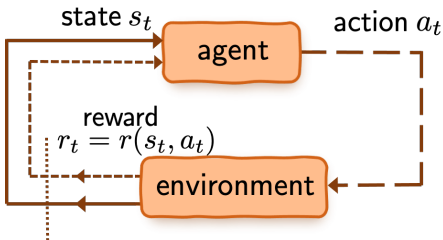
Example: grasping an object



RL **reinforces** the agents' decisions over time by observing the reward and state that result from taking different actions.

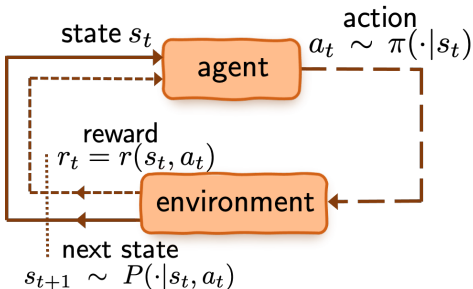
Markov decision processes

Infinite-horizon Markov decision process (MDP)



- \mathcal{S} : state space
- \mathcal{A} : action space
- $r(s, a) \in [0, 1]$: immediate reward

Infinite-horizon Markov decision process (MDP)



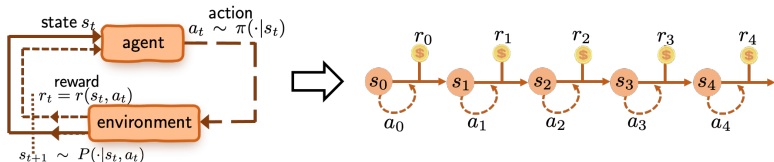
- \mathcal{S} : state space
- \mathcal{A} : action space
- $r(s, a) \in [0, 1]$: immediate reward
- $\pi(\cdot | s)$: policy (or action selection rule), deterministic or random
- $P(\cdot | s, a)$: transition probabilities

Help the mouse!



- state space \mathcal{S} : positions in the maze
- action space \mathcal{A} : up, down, left, right
- immediate reward r : cheese (+1), electricity shocks (-1), cats (-10000)
- policy $\pi(\cdot|s)$: the way to find cheese

Value function

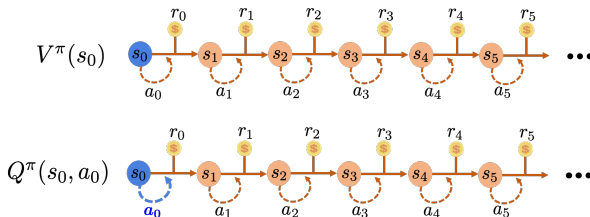


Value of policy π : cumulative **discounted** reward

$$\forall s \in \mathcal{S} : \quad V^\pi(s) := \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \mid s_0 = s \right]$$

- $(a_0, s_1, a_1, s_2, a_2, \dots)$: induced by policy π
- $\gamma \in [0, 1)$: discount factor,
 - γ close to 0 leads to **"myopic"** evaluation
 - γ close to 1 leads to **"far-sighted"** evaluation

Q-function (action-value function)



Q-function of policy π :

$$\forall (s, a) \in \mathcal{S} \times \mathcal{A}: \quad Q^\pi(s, a) := \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r_t \mid s_0 = s, a_0 = a \right]$$

- $(\cancel{a_0}, s_1, a_1, s_2, a_2, \dots)$: induced by policy π

Effective horizon

Since $r(s, a) \in [0, 1]$,

$$0 \leq V^\pi(s), Q^\pi(s, a) \leq \frac{1}{1 - \gamma}.$$

Often think of $\frac{1}{1 - \gamma}$ as the **effective horizon** of the problem.

Why Markov transitions?

- By the Markovian property,

$$\begin{aligned}P(s_{t+1}, s_t, \dots, s_0) &= P(s_0)P(s_1|s_0)P(s_2|s_1, s_0) \dots P(s_{t+1}|s_t, \dots, s_0) \\&= P(s_0)P(s_1|s_0)P(s_2|s_1, \cancel{s_0}) \dots P(s_{t+1}|s_t, \dots, \cancel{s_0}) \\&= P(s_0) \prod_{i=0}^t P(s_{i+1}|s_i).\end{aligned}$$

Low computation and memory complexity!

- The world is Markovian when the state space is large enough. For example, if $s_{t+1} \sim P(\cdot|s_t, s_{t-1})$ depends on the previous two steps, by working with $\tilde{s}_t = (s_t, s_{t-1})$ (and $s_{-1} = s_0$), we have

$$\tilde{s}_{t+1} \sim P(\cdot|\tilde{s}_t)$$

is Markovian.

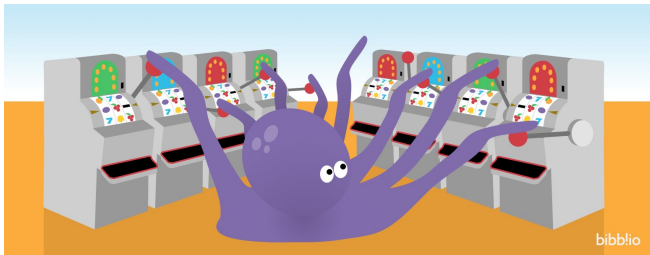
All models are wrong, but some are useful

Why discounting?



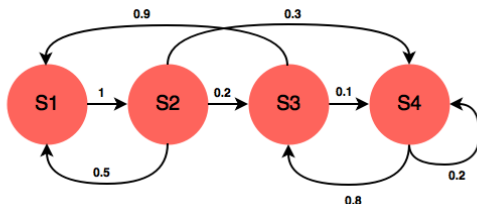
- Mathematically convenient: the limit always exists
- Immediate rewards earn more interest than future rewards
- Account for variability and uncertainty in the future which may not be fully captured
- Undiscounted MDP is possible, e.g. if all sequences terminate (like in a maze or game).
- Alternatives: average reward and finite-horizon episodic settings.

Reduction to multi-arm bandits



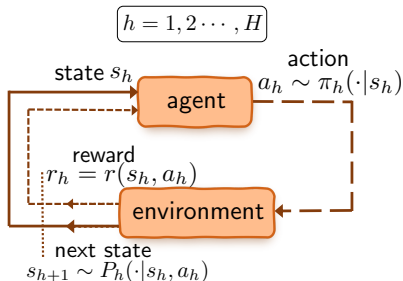
- No state transition: \mathcal{S} is a singleton
- The reward function is action-dependent (action = arm): $r(a)$
- Short-horizon planning: discount factor $\gamma = 0$
- The value of a policy π becomes $V^\pi := \mathbb{E}_\pi[r(a)]$.

Reduction to Markov reward process



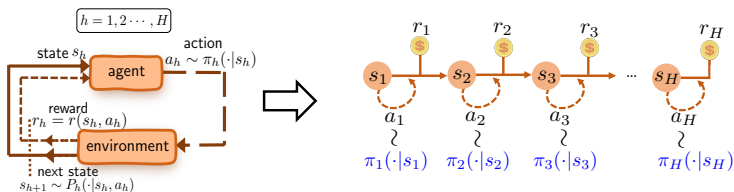
- No action selection: \mathcal{A} is a singleton
- The transition kernel defines a Markov chain
- The reward function is state-dependent: $r(s)$
- The value becomes $V(s) := \mathbb{E}_{\pi}[\sum_{t=0}^{\infty} \gamma^t r(s_t) \mid s_0 = s]$.

Finite-horizon episodic MDP



- H : horizon length
- \mathcal{S} : state space with size S
- \mathcal{A} : action space with size A
- $r_h(s_h, a_h) \in [0, 1]$: immediate reward in step h
- $\pi = \{\pi_h\}_{h=1}^H$: policy (or action selection rule)
- $P_h(\cdot | s, a)$: transition probabilities in step h

Value function and Q-function



$$V_h^\pi(s) := \mathbb{E} \left[\sum_{t=h}^H r_t(s_t, a_t) \mid s_h = s \right]$$

$$Q_h^\pi(s, a) := \mathbb{E} \left[\sum_{t=h}^H r_t(s_t, a_t) \mid s_h = s, a_h = a \right]$$



- execute policy π to generate sample trajectory

Basic tasks

Policy evaluation:

- given a policy π , how good is it?

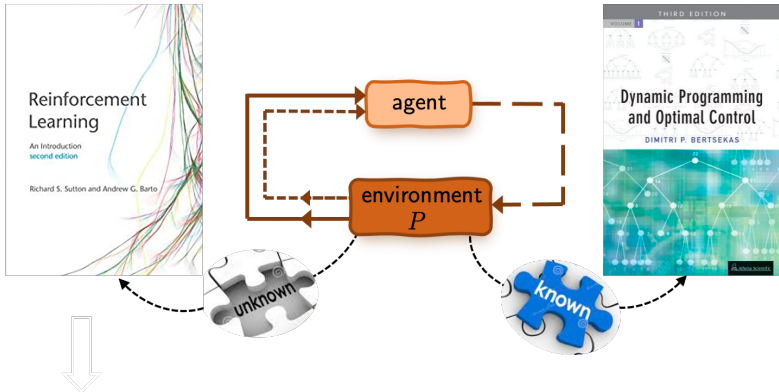
Policy improvements:

- given a policy π , can we find a better one?

Policy optimization:

- can we find the best policy for the given MDP?

Planning versus learning



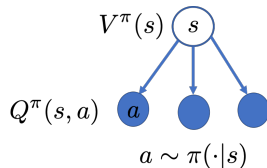
- **Planning:** solve for a desired policy given model specification
- **Learning:** learn a desired policy from samples w/o model specification

We'll focus on planning first.

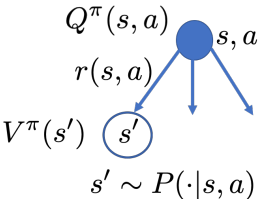
Policy evaluation

Policy evaluation: evaluating V via Q

$$\begin{aligned} V^\pi(s) &= \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \mid s_0 = s \right] \\ &= \sum_{a \in \mathcal{A}} \pi(a_0 = a \mid s = s_0) \underbrace{\mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \mid s_0 = s, a_0 = a \right]}_{=: Q^\pi(s, a)} \\ &= \mathbb{E}_{a \sim \pi(\cdot \mid s)} [Q^\pi(s, a)] \end{aligned}$$



Policy evaluation: evaluating Q via V

$$\begin{aligned}Q^\pi(s, a) &= \mathbb{E} \left[r(s, a) + \sum_{t=1}^{\infty} \gamma^t r(s_t, a_t) \mid s_0 = s, a_0 = a \right] \\&= \mathbb{E} [r(s, a)] + \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\mathbb{E} \left[\sum_{t=1}^{\infty} \gamma^t r(s_t, a_t) \mid s_1 = s', s_0 = s, a_0 = a \right] \right] \\&= \mathbb{E} [r(s, a)] + \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\mathbb{E} \left[\sum_{t=1}^{\infty} \gamma^t r(s_t, a_t) \mid s_1 = s' \right] \right] \\&= \mathbb{E} [r(s, a)] + \underbrace{\gamma \mathbb{E}_{s' \sim P(\cdot | s, a)} \left[\mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \mid s_0 = s' \right] \right]}_{=: V^\pi(s')} \\&= \mathbb{E} [r(s, a)] + \gamma \mathbb{E}_{s' \sim P(\cdot | s, a)} [V^\pi(s')]\end{aligned}$$


The diagram illustrates the relationship between the Q-value function $Q^\pi(s, a)$ and the V-value function $V^\pi(s')$ in policy evaluation. A blue circle at the top is labeled $Q^\pi(s, a)$ and s, a . Three arrows point downwards from this circle: one to a blue circle labeled $V^\pi(s')$ and s' , one to a label $r(s, a)$, and one to an unlabeled arrow. The $V^\pi(s')$ circle is also labeled $s' \sim P(\cdot | s, a)$.

Bellman's consistency equation

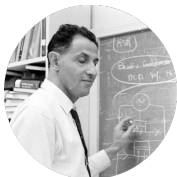
- V^π / Q^π : value / action-value function under policy π

Bellman's consistency equation

$$V^\pi(s) = \mathbb{E}_{a \sim \pi(\cdot|s)} [Q^\pi(s, a)]$$
$$Q^\pi(s, a) = \underbrace{\mathbb{E}[r(s, a)]}_{\text{immediate reward}} + \gamma \mathbb{E}_{s' \sim P(\cdot|s, a)} \left[\underbrace{V^\pi(s')}_{\text{next state's value}} \right]$$

The value/Q function can be decomposed into two parts:

- immediate reward $\mathbb{E}[r(s, a)]$
- discounted value of at the successor state $\gamma \mathbb{E}_{s' \sim P(\cdot|s, a)} V(s')$



Richard Bellman

Matrix-vector representation

- Plugging Q^π into V^π , we have

$$V^\pi(s) = \mathbb{E}_{a \sim \pi(\cdot|s)}[r(s, a)] + \gamma \mathbb{E}_{a \sim \pi(\cdot|s), s' \sim P(\cdot|s, a)}[V^\pi(s')].$$

- Let P^π be the state-state transition matrix induced by π , namely,

$$P^\pi(s'|s) = \sum_{a \in \mathcal{A}} \pi(a|s) P(s'|s, a).$$

- We can write the above in a matrix-vector form as

$$V^\pi = r^\pi + \gamma P^\pi V^\pi,$$

where $V^\pi = [V^\pi(s)]_{s \in \mathcal{S}}$, and $r = [\mathbb{E}_{a \sim \pi(\cdot|s)}[r(s, a)]]_{s \in \mathcal{S}}$.

a similar treatment applies to Q^π , too.

Solving the Bellman's consistency equation

$$V^\pi = r^\pi + \gamma P^\pi V^\pi \implies V^\pi = (I - \gamma P^\pi)^{-1} r^\pi$$

Invertibility of $I - \gamma P^\pi$: Gershgorin's circle theorem, or for any $x \in \mathbb{R}^{|\mathcal{S}|}$, verify

$$\begin{aligned} \|(I - \gamma P^\pi)x\|_\infty &\geq \|x\|_\infty - \gamma \|P^\pi x\|_\infty \\ &\geq \|x\|_\infty - \gamma \|x\|_\infty \quad (\|P^\pi x\|_\infty \leq \|P^\pi\|_1 \|x\|_\infty = \|x\|_\infty) \\ &\geq (1 - \gamma) \|x\|_\infty \\ &> 0. \end{aligned}$$

Thus, $I - \gamma P^\pi$ is full rank and invertible.

Computationally expensive for problems with large state space!

Bellman's policy operator

Bellman's policy operator: denote the operator $\mathcal{T}^\pi : \mathbb{R}^{|\mathcal{S}|} \mapsto \mathbb{R}^{|\mathcal{S}|}$ as

$$\forall V \in \mathbb{R}^{|\mathcal{S}|} : \quad \mathcal{T}^\pi(V) = r^\pi + \gamma P^\pi V.$$

Fixed-point equation:

$$V = \mathcal{T}^\pi(V)$$

- V^π is the unique fixed point of this fixed-point equation.

Contraction property of the Bellman's operator

Lemma 1

The operator \mathcal{T}^π is a γ -contraction on $\mathbb{R}^{|\mathcal{S}|}$, i.e. for any V and V' in $\mathbb{R}^{|\mathcal{S}|}$, it follows

$$\|\mathcal{T}^\pi(V) - \mathcal{T}^\pi(V')\|_\infty \leq \gamma \|V - V'\|_\infty.$$

Proof: For any V and V' ,

$$\begin{aligned}\|\mathcal{T}^\pi(V) - \mathcal{T}^\pi(V')\|_\infty &= \|\gamma P^\pi V - \gamma P^\pi V'\|_\infty \\ &\leq \gamma \|P^\pi\|_1 \|V - V'\|_\infty = \gamma \|V - V'\|_\infty,\end{aligned}$$

using $\|P^\pi\|_1 = 1$.

Fast computation without inversion

Value iteration for policy evaluation

For $t = 0, 1, 2, \dots$

$$V^{(t+1)} = \mathcal{T}^\pi(V^{(t)}).$$

Linear convergence:

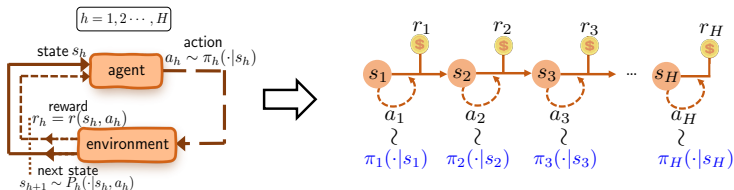
$$\begin{aligned}\|V^{(t+1)} - V^\pi\|_\infty &= \|\mathcal{T}^\pi(V^{(t)}) - \mathcal{T}^\pi(V^\pi)\|_\infty \\ &\leq \gamma \|V^{(t)} - V^\pi\|_\infty \\ &\leq \gamma^t \|V^{(0)} - V^\pi\|_\infty.\end{aligned}$$

Implication: to achieve $\|V^{(t+1)} - V^\pi\|_\infty \leq \epsilon$, it takes no more than

$$\frac{1}{1-\gamma} \log \left(\frac{\|V^{(0)} - V^\pi\|_\infty}{\epsilon} \right)$$

iterations.

Policy evaluation for finite-horizon MDPs



- 1 Begin with the terminal step $h = H + 1$:

$$V_{H+1}^\pi = 0, \quad Q_{H+1}^\pi = 0.$$

- 2 Backtrack $h = H, H - 1, \dots, 1$:

$$Q_h^\pi(s, a) := \underbrace{\mathbb{E}[r_h(s_h, a_h)]}_{\text{immediate reward}} + \underbrace{\mathbb{E}_{s' \sim P_h(\cdot | s, a)} V_{h+1}^\pi(s')}_{\text{next step's value}}$$

$$V_h^\pi(s) := \mathbb{E}_{a \sim \pi_h(\cdot | s)} Q_h^\pi(s, a)$$